

Conrad Stork

List of Publications by Year in descending order

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Version: 2024-02-01

18
papers

449
citations

932766

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839053

18
g-index

18
all docs

18
docs citations

18
times ranked

586
citing authors

#	ARTICLE	IF	CITATIONS
1	Skin Doctor CP: Conformal Prediction of the Skin Sensitization Potential of Small Organic Molecules. <i>Chemical Research in Toxicology</i> , 2021, 34, 330-344.	1.7	11
2	BonMOLiÃˆre: Small-Sized Libraries of Readily Purchasable Compounds, Optimized to Produce Genuine Hits in Biological Screens across the Protein Space. <i>International Journal of Molecular Sciences</i> , 2021, 22, 7773.	1.8	2
3	CYPstrate: A Set of Machine Learning Models for the Accurate Classification of Cytochrome P450 Enzyme Substrates and Non-Substrates. <i>Molecules</i> , 2021, 26, 4678.	1.7	5
4	Predicting the Skin Sensitization Potential of Small Molecules with Machine Learning Models Trained on Biologically Meaningful Descriptors. <i>Pharmaceuticals</i> , 2021, 14, 790.	1.7	7
5	CYPlebrity: Machine learning models for the prediction of inhibitors of cytochrome P450 enzymes. <i>Biorganic and Medicinal Chemistry</i> , 2021, 46, 116388.	1.4	16
6	Computational Applications in Secondary Metabolite Discovery (CAiSMD): an online workshop. <i>Journal of Cheminformatics</i> , 2021, 13, 64.	2.8	3
7	Computational prediction of frequent hitters in target-based and cell-based assays. <i>Artificial Intelligence in the Life Sciences</i> , 2021, 1, 100007.	1.6	3
8	NERDD: a web portal providing access to <i>in silico</i> tools for drug discovery. <i>Bioinformatics</i> , 2020, 36, 1291-1292.	1.8	46
9	ALADDIN: Docking Approach Augmented by Machine Learning for Protein Structure Selection Yields Superior Virtual Screening Performance. <i>Molecular Informatics</i> , 2020, 39, e1900103.	1.4	8
10	FAME 3: Predicting the Sites of Metabolism in Synthetic Compounds and Natural Products for Phase 1 and Phase 2 Metabolic Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3400-3412.	2.5	60
11	Skin Doctor: Machine Learning Models for Skin Sensitization Prediction that Provide Estimates and Indicators of Prediction Reliability. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4833.	1.8	15
12	NP-Scout: Machine Learning Approach for the Quantification and Visualization of the Natural Product-Likeness of Small Molecules. <i>Biomolecules</i> , 2019, 9, 43.	1.8	43
13	GLORY: Generator of the Structures of Likely Cytochrome P450 Metabolites Based on Predicted Sites of Metabolism. <i>Frontiers in Chemistry</i> , 2019, 7, 402.	1.8	57
14	Hit Dexter 2.0: Machine-Learning Models for the Prediction of Frequent Hitters. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 1030-1043.	2.5	70
15	Hit Dexter: A Machine Learning Model for the Prediction of Frequent Hitters. <i>ChemMedChem</i> , 2018, 13, 564-571.	1.6	34
16	PAIN(S) relievers for medicinal chemists: how computational methods can assist in hit evaluation. <i>Future Medicinal Chemistry</i> , 2018, 10, 1533-1535.	1.1	8
17	Why Are Dithienylethene-Linked Biscobaltocenes so Hard to Photoswitch?. <i>ChemPhysChem</i> , 2017, 18, 596-609.	1.0	5
18	FAME 2: Simple and Effective Machine Learning Model of Cytochrome P450 Regioselectivity. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 1832-1846.	2.5	56